Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electronic structure of the Sr/Si(001) Zintl template from density functional theory and photoemission HOSUNG SEO, MIRI CHOI, RICHARD HATCH, AGHAM POSADAS, ALEXANDER DEMKOV, The University of Texas at Austin — Since the first demonstration of epitaxial growth of crystalline SrTiO3 on Si(001) by Mckee and co-workers, sub-monolayer Sr on Si(001) has been extensively investigated. Charge transfer induced by half-monolayer of Sr has been shown to be a key element enabling wetting of Si by SrTiO3. However, a detailed understanding of the electronic structure reconstruction is not complete. Such knowledge could be extended and applied to the other epitaxial crystalline oxides on semiconductors. Recently, using in-situ x-ray core-level spectroscopy, we have studied the change in electronic structure of Si(001) induced by sub-monolayer Sr deposition in terms of surface core level shift. One of the interesting features is shift of the Si 2p level toward the higher binding energy by 0.49eV after Sr deposition. In this talk, we present a detailed theoretical investigation of the surface core level shifts in sub-monolayer Sr/Si(001). Using the final state theory, we calculate the bulk 2p binding energy to be increased by 0.42eV when half-monolayer of Sr is deposited in excellent agreement with experiment. We are able to compare the calculated evolution of the surface band structure in sub-monolayer Sr/Si(001) to angle-resolved photoemission spectroscopy (ARPES) data.

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Date submitted: 01 Nov 2012 Electronic form version 1.4